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PATENT


IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of: Dath et al
Serial No.: 09/205,056
Filed: December 3, 1998
Group Art Unit: 1764
Examiner: Nadine G. Norton
For: PRODUCTION OF PROPYLENE

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 Sheila Norman	January 27, 2003 Date of Deposit

Sir:

APPEAL BRIEF

This is an appeal from the decision of the Primary Examiner finally rejecting claims 15_ through 22. This Brief is submitted in triplicate.

Real Party in Interest

The real party in interest is Fina Research, S.A., a Belgium corporation, as recorded by the assignment dated March 2, 1999, and recorded in the Patent and Trademark Office on March 22, 1999, at Reel 9843 / Frame 0252.

Related Appeals and Interferences

There are presently no appeals or interferences directly related to this appeal. However, commonly-assigned applications having the same inventive entity as, or a common inventor with

this application and directed to catalytic cracking processes are the subjects of appeals as indicated below.

Application Serial No. 09/206,210; Notice of Appeal filed May 2, 2001

Application Serial No. 09/206,218; Notice of Appeal filed December 27, 2002

Application Serial No. 09/206,208; Notice of Appeal filed August 24, 2001

Application Serial No. 09/206,207; Notice of Appeal filed September 24, 2001

Application Serial No. 09/205,559; Notice of Appeal filed August 27, 2001

Application Serial No. 09/206,216; Notice of Appeal filed September 11, 2002

Application Serial No. 09/594,059; Notice of Appeal filed May 12, 2002

Application Serial No. 09/596,356; Notice of Appeal filed June 17, 2002

Status of Claims

The claims pending in this application are claims 15-22. No claim is allowed. Claims 15-22 are appealed and are reproduced in Exhibit A.

Status of Amendments

An Amendment Under 37 CFR 1.116 was filed on October 18, 2002 and entered by the advisory action of October 28, 2002.

Summary of the Invention

The invention called for in the claims on appeal involves a process for the production of propylene from an olefinic feedstock containing at least one olefin having four or more carbon atoms (last full paragraph on page 6). In carrying out the invention there is provided a crystalline silicate catalyst, specifically silicalite or ZSM-5, which has an MFI-type structure and contains aluminum and silicon in the catalyst framework to provide a silicon/aluminum atomic ratio. This

catalyst is subjected to a preliminary procedure which involves heating the catalyst in steam, followed by dealumination, in which the catalyst is contacted with a complexing agent for aluminum. This treatment removes amorphous aluminum produced during the steaming step from the catalyst framework and provides a catalyst of increased silicon/aluminum atomic ratio within the range of 180-1,000. The resulting catalyst is then contacted with the olefinic feedstock to produce an effluent containing propylene in which the propylene yield on an olefin basis is from 30%-50% based upon the olefinic content of the feedstock (paragraph bridging pp 12 and 14).

The MFI catalyst which is steamed and dealuminated to remove aluminum from the pores of the framework in accordance with appellants invention, is of a particular crystalline structure type as established by the Structure Commission of the International Zeolite Association, as referred to on page 1 of appellants' specification. As stated there, ZSM-5 and silicalite are MFI-type crystalline silicates. Attached hereto as Exhibit B is a copy of pages 1-12, and 89-93 from the *Atlas of Zeolite Structure Types* by Meier et al, published by the Structure Commission of the International Zeolite Association in 1978. As indicated on page 93, ZSM-5 and silicalite (referred to in Footnote 1 by reference to Flanigen et al (1978)) are MFI-structure types.

The effect of the steaming and dealumination procedure specified in appellants' claims is to remove aluminum from throughout the crystalline framework structure. This is described in the paragraph bridging pages 13 and 14 of the specification by reference to a typical commercially-available silicalite initially having a silicon/aluminum atomic ratio of about 120 (corresponding to a silica/alumina ratio of 240). The steaming step functions to reduce the tetrahedral aluminum in the crystalline framework to the form of amorphous alumina. The

subsequent treatment with the complexing agent functions to remove the amorphous alumina from the pores of the silicate framework so that dealumination occurs internally throughout the whole pore surfaces of the catalyst to increase the framework silicon/aluminum atomic ratio to a value of at least 180 (corresponding to a silica/alumina ratio of 360).

Prior Art

The prior art reference relied upon in rejecting the claims under 35 U.S.C. § 103 is EPO 19060 to Colombo.

Issues

The issues in this appeal are whether claims 15-21 are anticipated under 35 USC § 102(b) by EP 109060, and whether claims 15-22 are obvious under 35 USC § 103(a) over EP 109060.

Grouping of Claims

In the arguments presented in this Brief, all of the claims do not stand or fall together. In addition to the arguments made with respect to independent claim 15-20, additional arguments are made with respect to claims 21-22. Further, additional arguments are made with respect to each of independent claims 16, 17 and 18.

Appellants' Arguments

As the Examiner's position in rejecting the claims based upon EPO 109060 is understood, the Examiner appears to concede that reference fails to disclose or render obvious the process as set forth in claim 15 as involving subparagraphs a and b, or in claim 21 as involving subparagraphs a, b and c. However, the claimed subject matter is given no weight in determining the issue or novelty or unobviousness in view of the prior art on the grounds stated in the Final Rejection, at the bottom of page 3, that this involves "product by process limitations

which do not distinguish the claimed catalyst over the catalyst disclosed by the applied art.” Claims of 15-22 are not directed to a “claimed catalyst” and do not involve subject matter which can be characterized as product by process limitations, but instead positively recite a method for the production of polypropylene from an olefinic feed stock of at least one C₄+ olefin. The process as set forth in independent claim 15 involves the following:

the heating of the MFI silicate catalyst in steam,

de-aluminating the heated catalyst by treating the catalyst with a complexing agent for aluminum to remove aluminum from the catalyst framework and provide a catalyst of increased silicon/aluminum atomic ratio within the range of 180-1000,

and then contacting the pretreated catalyst with the olefinic feed stock to provide an effluent with a propylene yield of 30-50% based on the olefinic content of the feed stock.

Independent claim 21 calls for this process and further specifies that the steaming procedure reduces tetrahedral aluminum to form amorphous alumina followed by treatment with the complexing agent to remove amorphous alumina from the catalyst framework.

The fact that the claimed procedures are carried out prior to contacting of the catalyst with the olefinic feed stock does not detract from the fact that these are process limitations in process claims. The Manual of Patent Examining Procedure, makes clear that a lack of patentability under 35 U.S.C. 102 or 35 U.S.C. 103 cannot be established by simply ignoring claim limitations. Thus, as stated in MPEP Section 2116.01:

All the limitations of a claim must be considered when weighing the differences between the claimed invention and the prior art in determining the obviousness of a process or method claim. See MPEP § 2143.03. (emphasis original)

.....

Interpreting the claimed invention as a whole requires consideration of all claim limitations. Thus, proper claim construction requires treating language in a process claim, which recites the making or using of a nonobvious product as a material limitation.

MPEP § 2143.03 states:

“To establish prima facie obviousness of a claimed invention, all the claim limitations must be taught or suggested by the prior art. In re Royka, 490 F.2d 981, 180 USPQ 580 (CCPA 1974). “All words in a claim must be considered in judging the patentability of that claim against the prior art.” In re Wilson, 424 F.2d 1382, 1385, 165 USPQ 494, 496 (CCPA 1970).

Considering the mandate of the Manual of Patent Examining Procedure that all claim limitations must be considered and that lack of novelty or a prima facie case of obviousness can be established only when all of the limitations are taught by or obvious in view of the prior art, it becomes evident that claims 15 and 21 and the claims dependent thereon are neither anticipated by nor obvious in view of EP 109060.

The Final Rejection cites In re Marosi 218 USPQ 289 (Fed. Cir. 1983) and In re Thorpe (227 USPQ 964 (Fed. Cir. 1985)) to support this argument that subparagraphs (a) and (b) of claim 15 and (a), (b), and (c) of claim 21 should not be considered in evaluating patentability. However, it is respectfully submitted that these decisions do not support the proposition that process limitations in a process claim can be ignored. In fact, the Marosi decision clearly establishes the exact opposite. Thus, in Marosi, the court considered both process claims and product claims directed to a zeolite manufactured by the claimed process. The court, while affirming the rejection of the product by process claims, reversed the rejection of the process claims on the grounds that the prior art reference establishing a lack of patentability of the product by process claims did not render obvious the process itself. Hence, since claims 15-22

are process claims, embodying process limitations, it would appear that the decision cited by the Examiner supports patentability of these claims.

The Final Rejection at the top of page 4 acknowledges that EP '060 does not disclose the production of an effluent containing propylene in the effluent in an amount within the 30-50% range as specified in the claims 15 and 21. Instead, it is argued that this result of a propylene yield within the 30-50% range would be inherent in the operation of the reference. Appellants would respectfully disagree. The data presented in EP '060 for the various examples given there is somewhat sparse and is presented without elaboration. Thus, it is difficult to determine precisely what the propylene yield, in terms of the olefinic content of the feedstock, would be. However, one example, Example 36, does present in Fig. 1 the results of experimental work carried out employing Silicalite I as the catalyst and a feedstock of a 50/50 mixture of cis-butene-2 and trans-butene-2 over a period of 120 hours. While the silicon/aluminum atomic ratio of the Silicalite I of Example 36 is not given, it is noted that in the other examples employing silicalite, the silicon/aluminum ratio was necessarily greater than 1000. The results of Example 36 are presented in Fig. 1 of EP '060. As indicated there, the propylene content of the converted feed, as indicated by the selectivity to propylene, is less than 30% over the life of the run. The conversion of the olefinic feed ranges from about 68% to a maximum of about 80% initially and generally is about 75% until it starts to fall off after about 80 hours on stream. Throughout the test run, the propylene content (the product of conversion and selectivity) is clearly less than 25% based upon the olefinic content of the feedstock, which, of course, is 100%. Thus, based upon the data presented in Example 36, the conclusion clearly is that the propylene content is below the 30-50% range called for in appellants' claims.

Moreover, notwithstanding the data presented in Example 36 of EP '060, to the extent that the Final Rejection is based upon an argument of inherency, appellants would respectfully note that the law is well settled that for an alleged inherent feature to result from a prior art teaching, it is necessary that this inherent feature necessarily flow from the teachings of the prior art. Thus, an alleged inherent feature must be a necessary result and not merely a possible result. This principle is stated in MPEP Section 2112:

The fact that a certain result or characteristic may occur or be present in the prior art is not sufficient to establish the inherency of that result or characteristic. (Emphasis original)

Section 2112 reflects the general rule that for inherency to reside, it must be shown that the alleged inherency is necessarily present and not a mere possibility. Thus, as stated by the Board in *Ex parte Keith*, 154 USPQ 321 (Bd. of App. 1966), in reversing the Examiner's rejection based upon inherency:

There are other possible courses the reaction could follow . . . Asserted inherency must be a necessary result and not merely a possible result.

As indicated in Section 2112, this principle was more recently followed by the Board in *Ex parte Levy*, 17 USPQ2d 1461 (Bd. of App. and Interf. 1990), where the Board reversed an inherency rejection, stating as follows:

In relying upon the theory of inherency, the examiner must provide a basis in fact and/or technical reasoning to reasonably support the determination that the alleged inherent characteristic necessarily flows from the teachings of the prior art (citing cases). (emphasis original).

Here, the issue presented by the rejection based upon EP '060 is not only the requirement for a propylene yield of 30-50% but also the procedure in which the catalyst employed in cracking the olefinic feed stock be one which is pretreated by steaming and dealumination with a

complexing agent for aluminum to arrive at a catalyst in which the silicon/aluminum atomic ratio of the catalyst contacted with the feed stock is from 180 to 1,000. This combination of features is not disclosed or suggested in the EP '060 reference, and it is clearly not inherent therein.

In addition to the failure of the prior art to disclose the steaming and dealumination procedure, EP '060 does not disclose contacting an olefinic feedstock with an MFI-type catalyst having a silicon/aluminum atomic ratio of from 180 to 1000. EP '060 discloses a number of catalysts, some of which presumably are MFI-type catalysts and others which clearly are not. For example, EP '060 discloses the use of ZSM-5, silicalite (of a silica/alumina ratio well above the 180-1000 range), and ZSM-11. For the purpose of this appeal, it is presumed that the Silicalite I and the ZSM-5 zeolite disclosed in EP '060 are MFI crystalline silicates. Another catalyst disclosed in EP '060, ZSM-11, clearly is not an MFI-type silicate. In this regard, attention is respectfully invited to the aforementioned "Atlas of Zeolite Structure Types," attached as Exhibit B, and particularly the structure-type index appearing on pages 89-93 thereof. As shown there, ZSM-11 is of structure-type MEL. Various other catalysts disclosed in EP '060 may or may not be MFI-type zeolites; it is simply impossible to tell. The Silicalite 1 actually disclosed in EP '060 clearly does not have a silicon/aluminum atomic ratio of from 180 to 1000 as called for in appellants' claims. In fact, to the extent that the silicon/aluminum atomic ratio is addressed in EP '060, the reference simply requires a ratio of at least 175 and actually discloses an MFI-type catalyst (silicalite) in which no aluminum is present. In fact, every example in EP '060 addressing silicalite specifies a silicon/aluminum ratio of infinity, i.e. no aluminum is present. Thus, a fair reading of the disclosure in EP '060 is that the silicon/aluminum atomic ratio is of no significance, and it makes no difference whether or not aluminum is even present in the catalyst.

Referring to the dependent claims, dependent claim 16 calls for at least 95% of the C₃ compounds in the effluent to be propylene. Again referring to Example 36 as discussed above, it is noted that Fig. 1 discloses data over the course of the run for selectivity to liquids (C₅ and greater) and selectivity to saturated gases which presumably would include gases of less than C₅, specifically including propane. The selectivity to propylene is over most of the run about 7 to 8 times the selectivity to saturated gases, and thus it is clear that saturated C₃ content of the effluent could be well in excess of 5%, leaving the propylene content at less than 95%.

Dependent claim 17 specifies that the feedstock contacts the catalyst at an inlet temperature of 500-600°C. Dependent claim 18 specifies that the feedstock contacts the catalyst or is passed over the catalyst at a liquid hourly space velocity (LHSV) of from 10-30 h⁻¹. EP '060 does not disclose or suggest this particular combination of parameters and instead discloses, in addition to the very broad range of the silicon/aluminum ratio, broad ranges of olefin partial pressure, space velocity, and temperature. Thus, EP '060 specifies a temperature of 400-600°C and a space velocity of 5-200 hrs.⁻¹. Thus, while EP '060 discloses broad ranges of these parameters within which more specific values could be selected, the particular combination of the silicon/aluminum atomic ratio with the inlet temperature, as specified in claim 17, and space velocity, as set forth in claim 18, can be arrived at only by selecting these values from the broad ranges in EP '060 based upon appellants' disclosure. In fact, with respect to space velocity as set forth in dependent claim 18, the only qualification of space velocity as described in EP '060 appears to be that the space velocity should be less than 50 hrs.⁻¹ if the pressure is atmospheric and greater than 50 hrs.⁻¹ at a pressure of from 1.5 to 7.5 atmospheres. As a practical matter, EP '060 suggests as a whole that the space velocity should be outside the 10-30 hrs.⁻¹ range specified in appellants' dependent claim 18. An exception to this is found in the

aforementioned Example 36 of EP '060, but here a silicon/ aluminum atomic ratio of infinity (silicalite totally free of aluminum), rather than within the range of 180 to 1000, and a propylene yield well below the 30-50% value as called for in appellants' claims, are involved. There is simply nothing in EP '060 which discloses or renders obvious the combination of silicon/aluminum ratio, propylene yield, and space velocity as called for in the claims as indicated above.

As noted previously, claim 21 includes in addition to the procedure set forth in claim 15 calls for the requirement that the steaming procedure reduces tetrahedral aluminum to amorphous alumina which is removed by treatment with the complexing agent. Dependent claim at 22 specifies that the catalyst is silicalite and that it is heated in steam at a temperature within a range of 425-870°C. This subject matter clearly is not disclosed in or inherent in EPO 109060.

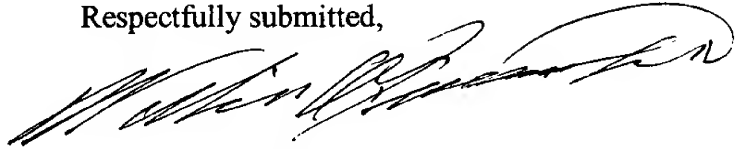
Conclusion

For the reasons set forth above, Appellants respectfully submit that all of the claims herein are patentable over the prior art. Accordingly, it is respectfully requested that the Final Rejection of the claims be reversed.

It is noted that this is the second appeal brief filed in this application with the requisite fee for filing a brief in support of appeal in accordance with 37 CFR § 1.17(c) being paid with the originally filed appeal brief. It is respectfully requested that the fee paid with the first appeal brief should be applied to this appeal in accordance with the procedure outlined in MPEP § 1208.03.

The Commissioner is hereby authorized to change any additional fees that may be due in connection with this appeal brief to Deposit Account No. 12-1781.

Respectfully submitted,

A handwritten signature in black ink, appearing to read 'William D. Jackson', with a large, stylized flourish at the end.

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EXHIBIT "A"

CLAIMS 15-22

15. A process for the production of propylene from an olefinic feedstock containing at least one olefin of C₄ or greater comprising:

(a) providing a crystalline silicate catalyst having an MFI structure and containing aluminum and silicon in the catalyst framework to provide a silicon/aluminum atomic ratio;

(b) subjecting said catalyst to a pretreatment procedure involving heating the catalyst in steam and de-aluminating the catalyst by treating the catalyst with a complexing agent for aluminum to remove aluminum from the catalyst framework and providing a catalyst of increased silicon/aluminum atomic ratio within the range of 180 to 1000; and

(c) contacting the pretreated catalyst with the olefinic feedstock containing at least one olefin of C₄ or greater to produce an effluent containing propylene in which the propylene yield on an olefin basis is from 30 to 50% based on the olefinic content of the feedstock.

16. A process according to claim 15, wherein at least 95 wt.% of any C₃ compounds in the effluent are present as propylene.

17. A process according to claim 15, wherein the feedstock contacts the catalyst at an inlet temperature of from 500 to 600°C.

18. A process according to claim 15, wherein the feedstock is passed over the catalyst at an LHSV of from 10 to 30h⁻¹.

19. A process according to claim 15, wherein the catalyst of the MFI structure is silicalite.

20. A process according to claim 15, wherein the catalyst of the MFI structure is ZSM-5.

21. A process for the production of propylene from an olefinic feedstock containing at least one olefin of C₄ or greater comprising:

(a) providing a crystalline silicate catalyst having an MFI structure and containing aluminum and silicon in the catalyst framework to provide a silicon/aluminum atomic ratio;

(b) subjecting said catalyst to a pretreatment procedure involving heating the catalyst in steam to reduce tetrahedral aluminum in the catalyst from the framework and form amorphous alumina in the pores of the catalyst;

(c) de-aluminating the catalyst by treating the catalyst with a complexing agent for aluminum to remove amorphous alumina from the catalyst framework and provide a catalyst of increased silicon/aluminum atomic ratio within the range of 180 to 1000; and

(d) contacting the pretreated catalyst with the olefinic feedstock containing at least one olefin of C₄ or greater to produce an effluent containing propylene in which the

propylene yield on an olefin basis is from 30 to 50 wt.% based on the olefinic content of the feedstock.

22. The process of claim 21 wherein said catalyst is silicalite and is heated in steam to a temperature within the range of 425°-870°C.

Exhibit B

ATLAS OF ZEOLITE STRUCTURE TYPES

by

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Structure type data sheets with stereopairs (in alphabetical order according to the structure type codes)

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ABW	AFG	ANA	BK
BRE	CAN	CHA	DAC
EAB	EDI	EPI	ERI
FAU	FER	GIS	GME
HEU	KFI	LAU	LEV
LIO	LOS	LTA	LTL
MAZ	MEL	MER	MFI
MOR	NAT	OFF	PAU
PHI	RHO	SOD	STI
THO	YUG		

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89

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PREFACE

The steadily growing number of known zeolite structures and numerous requests which have been received for a previous survey of zeolite framework types has led to the present "Atlas of Zeolite Structure Types". The primary aim of the present compilation is to define and to supply a condensed characterization of the 38 currently established zeolite structure types. Apart from the stereopairs illustrating the framework structures the Atlas contains summaries of structural data as well as a Structure Type Index that includes all natural and synthetic materials which have been shown to be an isotype of a known zeolite structure type.

The present Atlas contains only reasonably well-established structures which have been at least partially refined. A number of zeolite structures included are by necessity based on powder data. A total of 38 structure types could, after critical assessment of the respective structure analysis, be included in this Atlas (compared to 27 in the previous survey by Meier and Olson, 1971).

Zeolites do not comprise an easily definable family of crystalline aluminosilicates. The inclusion or exclusion of borderline cases was decided on the basis of criteria used at recent International Conferences on zeolites.

We wish to acknowledge the use of the stereographic computer plotting program ORTEP, written by Dr. Carroll K. Johnson (Oak Ridge National Laboratory). A listing of the ORTEP input used to generate the stereopairs in this Atlas has been deposited as document number NAPS-03331. (Order from ASIS/NAPS, Microfilm Publications, P. O. Box 3513, Grand Central Station, New York, N. Y. 10017). Information obtained by private communication in addition to the published data has in several instances been used in the preparation of the Atlas. Such use is indicated in the References and we gratefully acknowledge this help. We also wish to thank our colleagues of the IZA Structure Commission for critically

reading the manuscript and many helpful comments. Furthermore, we are grateful for the support by Mobil Research and Development Corporation and one of us (D. K. O.) is also indebted to this company for permission to participate in this project. The work of the other author (W. M. M.) has been part of a research program supported by the Swiss National Science Foundation.

Explanatory Notes

Probably the simplest way of illustrating zeolite structures is by means of skeletal models or diagrams showing the 4-connected nets formed by the tetrahedral atoms in the various aluminosilicate frameworks. The known zeolite framework types are presented in this Atlas by means of stereographic drawings of this kind. In general, the viewing direction (which is stated in each case) has been chosen in such a way that the main channels are clearly visible. The unit cell has also been outlined whenever possible and provided that no changes in symmetry affecting the cell edges have been encountered. The positions of atoms (T = Si, Al) are those of the points or vertices of the net and the T-O-T bridges are represented by straight lines. The positions of the O-atoms are only approximately displayed in these diagrams since the T-O-T angles are typically around $140-150^\circ$. The idealization makes it easier to visualize the topology and basic features of zeolite framework structures which in many instances are relatively complex.

STRUCTURE TYPE

Structural classifications of zeolites are primarily based on the topology of the frameworks. Zeolite species which do not differ with respect to the framework topology are called isotypic, i.e. they refer to the same structure type irrespective of composition, distribution of the different T-atoms, cell dimensions, and symmetry. A mnemonic code consisting of 3 capital letters has been adopted for each structure type following the recommendations by IUPAC on zeolite nomenclature¹⁾.

1) "Chemical Nomenclature, and Formulation of Compositions, of Synthetic and Natural Zeolites", prepared by a special IUPAC Commission under the chairmanship of R. M. Barrer. IUPAC yellow booklet, 1978.

Structure type codes are generally derived from the names of the type species (see below) and do not include numbers and characters other than capital roman letters. Since structural criteria alone do not provide an unambiguous numbering scheme, and to facilitate later additions and simple indexing, the various structure types in this Atlas have been arranged in alphabetical order according to the structure type code. For each structure type the information given in bold type includes the full type name, the maximum topological symmetry (i.e. the maximum possible space group) and a listing of the topologically distinct T-atoms, their number per unit cell, as well as the maximum point symmetry of the respective T-sites (in square parentheses).

Secondary Building Units (SBU)

Zeolite frameworks can be thought to consist of finite or infinite (i.e. chain- or layer-like) component units. The finite units containing up to 16 T-atoms, which have been found to occur in framework silicates, are shown in Figure 1. These secondary building units¹⁾ are derived²⁾ assuming the entire framework is made up of one type of SBU only. A unit cell invariably contains an integral number of SBU. Many of the frameworks can be built from several different SBU. In these cases the SBU listed in the first place is the one which occurs most frequently in related structures.

- 1) The primary building units being the single TO_4 tetrahedra.
- 2) There is evidence, however, that some zeolite frameworks consist of two component units, such as 4-membered rings of silica tetrahedra which are linked to each other through single AlO_4 tetrahedra as in the case of laumontite and (possibly) analcime.

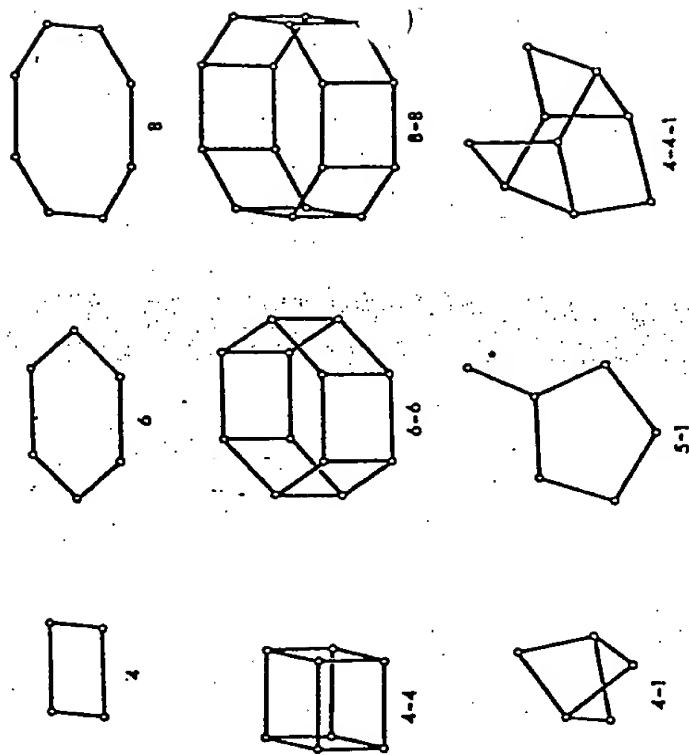


Figure 1

Framework Density (FD)

This is defined as the number of T-atoms per 1000 \AA^3 . For most zeolite framework structures values of at least $20 \text{ T}/1000 \text{ \AA}^3$ are generally obtained while for zeolites the observed values range from about 10 for structures with the largest pore volume to around 20. The FD is obviously related to the pore volume but does not reflect the size of the pore openings. For some non-rigid zeolite structure types the FD values can vary appreciably. In these cases (such as glauconite) values are given for the type species and the framework in the most expanded state. The flexibility of the framework structure is to some extent displayed by the possible variation of the FD.

orthand notation has been adopted for the description of the channels in the various frameworks. Each system of equivalent channels has been characterized by the channel direction (relative to the axes of the type structure) the number of either T- or O-atoms (underlined number) forming the smallest rings of the channels, and the crystallographic free diameters of the channels.

Free diameter values are based on the atomic coordinates of the species in the hydrated state and an oxygen radius of 1.35 Å. Minimum and maximum values are given for non-circular apertures. In many instances the corresponding interatomic distance vectors are approximately co-planar, and closer inspection of the diagrams will give some information on this in the first instance. It should be noted that crystallographic free diameters depend on the state of composition of the zeolite, and can differ appreciably for various zeolite species, particularly in the case of non-rigid frameworks.

The number of asterisks in the notation used indicates whether the channel system is one-, two- or three-dimensional. Only those apertures have been taken into account which are more open than regular six-membered rings. In most cases these smaller openings simply form windows (rather than channels) connecting larger cavities. Interconnected channel systems are separated by a double arrow (\longleftrightarrow). A vertical bar (|) means that there is no direct access from one channel system to the other.

The selected examples in Table 1 illustrate the various possibilities in the use of the notation. Cancrinite is characterized by a one-dimensional system of channels parallel to $[001]$ or \underline{c} with circular ring apertures. In offretite the main channels form a similar system and are interconnected by channels made of 8-rings giving rise to a

3-dimensional channel system. The channel system in mordenite is essentially 2-dimensional, the 12-ring apertures of the main channels being somewhat elliptical. Paulingite is an example of a framework type containing two independent sets of 3-dimensional channel systems which are displaced against each other. ($\langle 100 \rangle$ means there are channels parallel to all crystallographically equivalent axes of the cubic structure, i.e. along \underline{x} , \underline{y} and \underline{z}). In glismondine the channels parallel to $[100]$ together with those parallel to $[010]$ give rise to a 3-dimensional channel system which can be pictured as an array of partially overlapping tubes.

Table 1: EXAMPLES ILLUSTRATING THE NOTATION FOR THE CRYSTALLOGRAPHIC CHARACTERIZATION OF THE CHANNEL

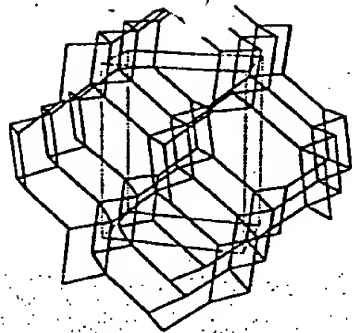
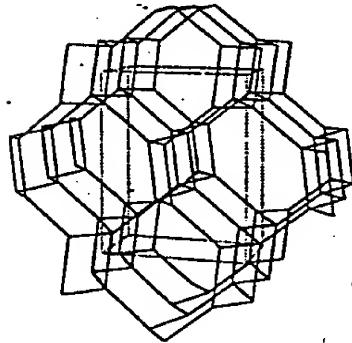
Cancrinite	$[001] \quad \underline{12} \quad 6.2^*$
Offretite	$[001] \quad \underline{12} \quad 6.4^* \longleftrightarrow \perp [001] \quad \underline{8} \quad 3.6 \times 5.2^{**}$
Mordenite	$[001] \quad \underline{12} \quad 6.7 \times 7.0^* \longleftrightarrow [010] \quad \underline{8} \quad 2.9 \times 5.7^*$
Paulingite	$\langle 100 \rangle \quad \underline{8} \quad 3.9^{***} \mid \langle 100 \rangle \quad \underline{8} \quad 3.9^{***}$
Glismondine	$\{ [100] \quad \underline{8} \quad 3.1 \times 4.4 \longleftrightarrow [010] \quad \underline{8} \quad 2.8 \times 4.9 \}^{***}$

Fault Planes (FP)

Likely FP are listed for each structure type. The existence of FP means that layer-like segments of the framework can be stacked in more than one way, giving rise to polytypism. A number of related structures (polytypes) can be readily postulated on this basis. FP also serve as an indication of possible stacking faults which may affect the critical channel dimensions.

Type Species and References

The type species stated in the data section is the species used to establish the structure type. In the majority of cases these have been natural zeolites providing single crystal data. The composition expressed in terms of cell contents has in many cases been idealized inasmuch as compositional data give average unit cell contents which frequently correspond to fractional numbers of atoms. Isotypic species are very common and have been listed in the Index.



Li-A(BW)

Imam

8 T[m

viewed along [001]

Secondary building units:

single 4-rings
(single 6- or 8-rings)

Framework density:

19.0 T/1000 Å³

Channels:

[001] 8 3.6 x 4.0 *

Fault planes:

(010), (011)

Type species:

synthetic zeolite Li-A (Barrer + White)

Li₄Al₄Si₄O₁₆ · 4 H₂O

orthorhombic, Pna2₁, a=10.3 b=8.2 c=5.0 Å³

References:

¹⁾ I. S. Kerr (1974)

Structure Type Index

Type species are marked by an asterisk. To make the index as informative as possible all reported species and designations have been included in this section, provided the structure type assignment appears reasonably well established. Even a number of occasionally used but discredited names of mineral species have been included in this index for the afore-mentioned reason. Moreover, the inclusion of a synthetic species designation in this index must not be interpreted to mean that the designation has been formally recognized or generally accepted but merely that the material has one of the established structure types. References have been restricted to those considered necessary to identify the species. For unreference minerals, see Strunz (1977).

* Afghanite	AFG	G. T. Wadlinger, E. J. Rosinski, and C. J. Plank (1968)
ALPHA	LTA	
A, Na-A	LTA	D. W. Breck, W. G. Eversole, R. M. Milton, T. B. Reed and T. L. Thomas (1956)
* Analcime	ANA	
— Analcite	ANA	
B	GIS	R. M. Milton (1961)
Ba-G	LTL	R. M. Barrer and D. J. Marshall (1964)
Ba-P	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
Ba-Q	KFI	R. M. Barrer, L. Hinds and E. A. D. White (1953)
Barrerite	STI	E. Passaglia and D. Pongiluppi (1975)
Basic cancrinite	CAN	R. M. Barrer and E. A. D. White (1952)
Basic sodalite	SOD	R. M. Barrer and E. A. D. White (1952)
* Bikitaitite	BIK	
* Brewsterite	BRE	

Ca-D	ANA	L. L. Ames and L. B. Sand (1958)
Cancrinite	CAN	
Cancrinite hydrate	CAN	J. Wyart and Michel-Lévy (1949)
Chabazite	CHA	
Clinoptilolite	HEU	A. Alberti (1975)
CsAlSiO ₄	ABW	S. J. Chung and Th. Hahn (1972)
D	CHA	D. W. Beck and N. A. Acara (1960)
Dachiardite	DAC	
Danellite	SOD	
Desmine	STI	
Edingtonite	EDI	
Epidesmine	STI	
Eplstibite	EPI	
Erlonite	ERI	
Faujasite	FAU	
Ferrierite	FER	
Garronite	GIS	G. P. L. Walker (1962)
Gismondine	GIS	
Gmelinite	GME	
Gonnardite	THO	
Harmotome	PHI	
Herschelite	CHA	
Heulandite	HEU	
Hydroxysodalite	SOD	W. Borchert and J. Heldel (1947)
(K, Ba) -G	LTL	R. M. Barrer and D. J. Marshall (1964)
Keholte	ANA	D. McConnell (1964)
K-F	EDI	R. M. Barrer and J. W. Baynham (1956)
K-M	MER	R. M. Barrer and J. W. Baynham (1956)
Laubandite	NAT	
Laumontite	LAU	
Leucite	ANA	

Leonhardite	LAU	C. T. Amirov, V. V. Dyukhin and N. V. Belov (1967)
* Levyne	LEV	
Levynite	LEV	
* Li-A	ABW	R. M. Barrer and E. A. D. White (1951)
* Linde A	LTA	D. W. Breck, W. G. Eversole, R. M. Milton, T. B. Reed and T. L. Thomas (1958)
Linde B	GIS	R. M. Milton (1961)
Linde D	CHA	D. W. Breck and N. A. Acara (1960)
* Linde L	LTL	D. W. Breck (1965)
Linde R	CHA	D. W. Breck and E. M. Flanigen (1968)
Linde T	OFF-ERI	R. M. Milton (1960)
Linde W	MER	D. W. Breck and N. A. Acara (1960)
Linde X	FAU	R. M. Milton (1961)
Linde Y	FAU	R. M. Milton (1959)
* Liottite	LIO	D. W. Breck (1964)
* Losod	LOS	W. Sieber and W. M. Meier (1974)
* Mazzite	MAZ	
* Merlinoite	MER	
* Mordenite	MOR	
N-A	LTA	R. M. Barrer and P. J. Denny (1961)
Na-B	ANA	R. M. Barrer and E. A. D. White (1952)
Na-D	MOR	R. M. Barrer and E. A. D. White (1952)
Na-P1	GIS	R. M. Barrer, F. W. Bultitude and I. S. Kerr (1959)
Na-P2	GIS	R. M. Barrer, F. W. Bultitude and I. S. Kerr (1959)
* Natrolite	NAT	
Nosean	SOD	
O	OFF	R. Alelio and R. M. Barrer (1970)
* Offretite	OFF	
Omega	MAZ	E. M. Flanigen (1968)
* Paulingite	PAU	

P-[Cl]	KFI	R.M. Barrer, L. Hinds and E.A.D. White (1953)
P _c , P _t	GIS	A.M. Taylor and R. Roy (1964)
* Phillipsite	PHI	
P-L	LTL	E.M. Flanigen and R.W. Grose (1971)
P, Na-P	GIS	R.M. Barrer, J.W. Baynham, F.W. Bultitude, and W.M. Meier (1959)
Pollucite	ANA	
Ptilolite	MOR	
Q-[Br]	KFI	R.M. Barrer, L. Hinds and E.A.D. White (1953)
R	CHA	R.M. Milton (1960)
RbAlSiO ₄	ABW	S.J. Chung and Th. Hahn (1972)
* Rho	RHO	H.E. Robson, D.P. Shoemaker, R.A. Oglvie and P.C. Manor (1973)
Scolecite	NAT	
S, Na-S	GME	R.M. Barrer, J.W. Baynham, F.W. Bultitude and W.M. Meier (1959)
* Sodallite	SOD	
Sodalite hydrate	SOD	J. Wyart and M. Michel-Lévy (1949)
Sr-D	FER	R.M. Barrer and D.J. Marshall (1964)
Sr-Q	YUG	R.M. Barrer and D.J. Marshall (1964)
Stellerite	STI	
* Stilbite	STI	
T	OFF-ERI	D.W. Breck and N.A. Acara (1960)
Tetracalcium trialuminate	SOD	V.I. Ponomarev, D.M. Khelker and N.V. Belov (1970)
* Thomsonite	THO	
* TMA-E	EAB	R. Aiello and R.M. Barrer (1970)
Tugtupite	SOD	H. Sorensen (1963)
Ultramarine	SOD	
Vlaelie	ANA	J. Mélon (1942)

W	MER	R.M. Milton (1961)
Wairakite	ANA	A. Steiner (1955)
Wellsite	PHI	P. Cerny, R. Rinaldi and R.C.S. dam (1977)
X	FAU	R.M. Milton (1959)
Y	FAU	D.W. Breck (1964)
* Yugawaralite	YUG	
Zeolon	MOR	
Zh	SOD	S.P. Zhdanov and N.N. Buntar (1971)
ZK-4	LTA	G.T. Kerr (1966)
* ZK-5	KFI	G.T. Kerr (1963)
ZK-19	PHI	G.H. Kuhl (1969)
ZK-20	LEV	G.T. Kerr (1969)
ZK-21	LTA	G.H. Kuhl (1967, 1971)
ZK-22	LTA	G.H. Kuhl (1967, 1971)
ZSM-4	MAZ	J. Ciric (1967)
* ZSM-5 ¹⁾	MFI	R.J. Argauer and G.R. Landolt (1972)
* ZSM-11	MEL	P. Chu (1973)

¹⁾ Recently, E.M. Flanigen et al (1978) reported a silica polymorph having the MFI structure type.